

NAG Library Routine Document

C06REF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

C06REF computes the discrete Fourier sine transforms of m sequences of real data values. The elements of each sequence and its transform are stored contiguously.

2 Specification

SUBROUTINE C06REF (M, N, X, IFAIL)

INTEGER M, N, IFAIL

REAL (KIND=nag_wp) X(N-1,M)

3 Description

Given m sequences of $n-1$ real data values x_j^p , for $j = 1, 2, \dots, n-1$ and $p = 1, 2, \dots, m$, C06REF simultaneously calculates the Fourier sine transforms of all the sequences defined by

$$\hat{x}_k^p = \sqrt{\frac{2}{n}} \sum_{j=1}^{n-1} x_j^p \times \sin\left(jk\frac{\pi}{n}\right), \quad k = 1, 2, \dots, n-1 \text{ and } p = 1, 2, \dots, m.$$

(Note the scale factor $\sqrt{\frac{2}{n}}$ in this definition.)

This transform is also known as type-I DST.

Since the Fourier sine transform defined above is its own inverse, two consecutive calls of C06REF will restore the original data.

The transform calculated by this routine can be used to solve Poisson's equation when the solution is specified at both left and right boundaries (see Swarztrauber (1977)).

The routine uses a variant of the fast Fourier transform (FFT) algorithm (see Brigham (1974)) known as the Stockham self-sorting algorithm, described in Temperton (1983), together with pre- and post-processing stages described in Swarztrauber (1982). Special coding is provided for the factors 2, 3, 4 and 5.

4 References

Brigham E O (1974) *The Fast Fourier Transform* Prentice–Hall

Swarztrauber P N (1977) The methods of cyclic reduction, Fourier analysis and the FACR algorithm for the discrete solution of Poisson's equation on a rectangle *SIAM Rev.* **19**(3) 490–501

Swarztrauber P N (1982) Vectorizing the FFT's *Parallel Computation* (ed G Rodrique) 51–83 Academic Press

Temperton C (1983) Fast mixed-radix real Fourier transforms *J. Comput. Phys.* **52** 340–350

5 Arguments

1: M – INTEGER

Input

On entry: m , the number of sequences to be transformed.

Constraint: $M \geq 1$.

- 2: N – INTEGER *Input*
On entry: one more than the number of real values in each sequence, i.e., the number of values in each sequence is $n - 1$.
Constraint: $N \geq 1$.
- 3: X(N – 1, M) – REAL (KIND=nag_wp) array *Input/Output*
On entry: the data values of the p th sequence to be transformed, denoted by x_j^p , for $j = 1, 2, \dots, n - 1$ and $p = 1, 2, \dots, m$, must be stored in $X(j, p)$.
On exit: the $(n - 1)$ components of the p th Fourier sine transform, denoted by \hat{x}_k^p , for $k = 1, 2, \dots, n - 1$ and $p = 1, 2, \dots, m$, are stored in $X(k, p)$, overwriting the corresponding original values.
- 4: IFAIL – INTEGER *Input/Output*
On entry: IFAIL must be set to 0, –1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.
For environments where it might be inappropriate to halt program execution when an error is detected, the value –1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this argument, the recommended value is 0. **When the value –1 or 1 is used it is essential to test the value of IFAIL on exit.**
On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, $M = \langle \text{value} \rangle$.
Constraint: $M \geq 1$.

IFAIL = 2

On entry, $N = \langle \text{value} \rangle$.
Constraint: $N \geq 1$.

IFAIL = 3

An internal error has occurred in this routine. Check the routine call and any array sizes. If the call is correct then please contact NAG for assistance.

IFAIL = –99

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL = –399

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -999

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

Some indication of accuracy can be obtained by performing a subsequent inverse transform and comparing the results with the original sequence (in exact arithmetic they would be identical).

8 Parallelism and Performance

C06REF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

The time taken by C06REF is approximately proportional to $nm \log(n)$, but also depends on the factors of n . C06REF is fastest if the only prime factors of n are 2, 3 and 5, and is particularly slow if n is a large prime, or has large prime factors. Workspace of order $O(n)$ is internally allocated by this routine.

10 Example

This example reads in sequences of real data values and prints their Fourier sine transforms (as computed by C06REF). It then calls C06REF again and prints the results which may be compared with the original sequence.

10.1 Program Text

```

Program c06refe

!      C06REF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
Use nag_library, Only: c06ref, nag_wp
!      .. Implicit None Statement ..
Implicit None
!      .. Parameters ..
Integer, Parameter          :: nin = 5, nout = 6
!      .. Local Scalars ..
Integer                     :: ieof, ifail, j, m, n, n1
!      .. Local Arrays ..
Real (Kind=nag_wp), Allocatable :: x(:, :)
!      .. Executable Statements ..
Write (nout,*) 'C06REF Example Program Results'
!      Skip heading in data file
Read (nin,*)
loop: Do
    Read (nin,*,Iostat=ieof) m, n1
    n = n1 + 1
    If (ieof<0) Then
        Exit loop
    End If

    Allocate (x(n1,m))
    Read (nin,*)(x(1:n1,j),j=1,m)
    Write (nout,*)

```

```

      Write (nout,*) 'Original data values'
      Write (nout,*)
      Write (nout,99999)(x(1:n1,j),j=1,m)

!      ifail: behaviour on error exit
!      =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
      ifail = 0
!      -- Compute transform
      Call c06ref(m,n,x,ifail)

      Write (nout,*)
      Write (nout,*) 'Discrete Fourier sine transforms'
      Write (nout,*)
      Write (nout,99999)(x(1:n1,j),j=1,m)

!      -- Compute inverse transform
      Call c06ref(m,n,x,ifail)

      Write (nout,*)
      Write (nout,*) 'Original data as restored by inverse transform'
      Write (nout,*)
      Write (nout,99999)(x(1:n1,j),j=1,m)
      Deallocate (x)
End Do loop

99999 Format (1X,5F10.4)
      End Program c06refe

```

10.2 Program Data

C06REF Example Program Data

```

3      5      : m, n-1
0.6772 0.1138 0.6751 0.6362 0.1424
0.2983 0.1182 0.7255 0.8638 0.8723
0.0644 0.6037 0.6430 0.0428 0.4815 : x

```

10.3 Program Results

C06REF Example Program Results

Original data values

0.6772	0.1138	0.6751	0.6362	0.1424
0.2983	0.1182	0.7255	0.8638	0.8723
0.0644	0.6037	0.6430	0.0428	0.4815

Discrete Fourier sine transforms

1.0014	0.0062	0.0834	0.5286	0.2514
1.2478	-0.6598	0.2570	0.0858	0.2658
0.8521	0.0719	-0.0561	-0.4890	0.2056

Original data as restored by inverse transform

0.6772	0.1138	0.6751	0.6362	0.1424
0.2983	0.1182	0.7255	0.8638	0.8723
0.0644	0.6037	0.6430	0.0428	0.4815
